



## Unsteady flame/vortex interactions studied

The importance of flame/vortex interactions in turbulent nonpremixed flames is well known. In particular, the presence of vortices near the flame surface induce flame curvature and unsteady strain rates that can lead to local flame extinction. Robert Schefer and Chuck Mueller have used planar, laser-induced fluorescence (PLIF) imaging to better understand the effect of these interactions on flame structure.

The burner (Figure 1) consists of a planar, laminar methane jet surrounded by a lower velocity coflow air stream. The test section is a 150-mm square chamber with quartz windows on two sides that provide optical access. A two-dimensional flame is produced with identical flame sheets located in the mixing layers adjacent to the fuel jet. Vortices are introduced by applying an impulse to loudspeakers attached to the side walls of the fuel-jet duct. These two-dimensional vortices provide a highly-reproducible interaction with the flame sheets.

Four representative images showing the time development of the flame/vortex interaction are presented in Figure 2. Here acetone seeded into the fuel flow was used as a fuel tracer. The acetone PLIF images, indicated by the blue-yellow false-color map, have been superimposed on the OH images, indicated by the orange-color map, to better define the flame/vortex relationship. The flame is lifted at a constant height of about 5 mm above the fuel nozzle exit. At this forcing frequency the close vortex spacing prevents the flame from attaching to the fuel nozzle. Most notable is the extinction of the OH layer along the upstream vortex edge. At time  $t = 0$ , the OH layer thickness is nearly constant along the downstream

edge of the upstream vortex. During the next two images the OH layer is stretched and thinned until a break occurs in this region. This event results in the formation of a separated island of OH that subsequently burns out.

The superimposed acetone images reveal the presence of two fuel-side vortices that cause local extinction of the OH layer. One vortex, located above the rolled-up portion of the flame and rotating clockwise, accounts for the large curvature produced as the OH layer wraps around it. A second vortex, located upstream of the flame, is smaller and again rotates clockwise. It also has a higher speed and thus moves closer to the downstream vortex during the sequence. The locally fuel-rich gas composition, in combination with the high strain induced by the rotational motion of the vortices, eventually quenches the OH where the distance between vortices is minimum.

Future work will extend measurements in the forced, planar jet to include velocity, methane concentration, and temperature, which will allow characterization of the effects of flow unsteadiness on flame chemistry and provide a basis for comparison with the modeling calculations of Habib Najm.

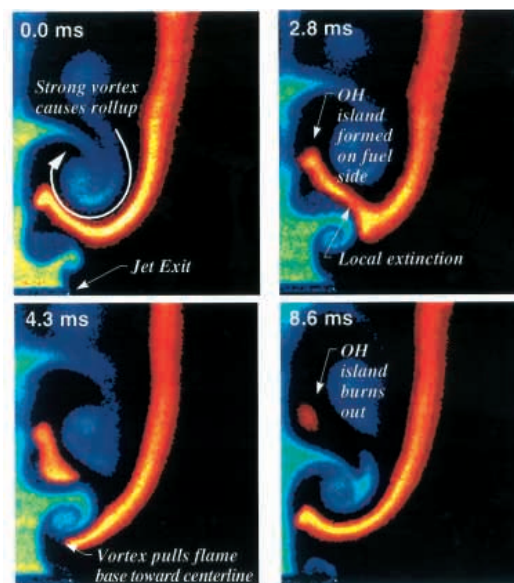


Figure 2. Time sequence of OH PLIF images at 90 Hz forcing frequency. Each false-color image covers a field-of-view 29.3 mm in the horizontal direction by 34.9 mm in the vertical, with only the right side of the flame shown. Upper left image is defined as  $t=0$ .



The CRF recently hosted Del Raymond and Judy Kieffer, Weyerhaeuser Company, for a day of technical discussions of research needs by the U.S. pulp and paper industry. Del is the Director of Strategic Energy Alternatives at Weyerhaeuser and Chairman of the Chief Technical Officers Committee of the American Forest & Paper Association, which is working with DOE/Office of Industrial Technologies to manage OIT's Industries of the Future projects related to pulp and paper manufacturing. Judy assists in the management of the program. Del gave an invited review of his perspective on research needs in his industry to a lively audience. Shown in the photo are (left to right) Don Hardesty, Larry Baxter, Del, Bob Gallagher, Judy, and Bill McLean.



Stephen Klippenstein (left), Professor of Chemistry at Case Western Reserve University, spent the month of July with Jim Miller, working on hindered rotor effects on elementary reactions in combustion.

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**Director:** William J. McLean  
Mail Stop 9054, (925) 294-2687

**Editor:** Lizbette Cox  
Mail Stop 9056, (925) 294-2322  
lrcox@Sandia.gov

Photographs of the 1998 summer visitors to the CRF can be found at [www.ca.sandia.gov/crf/WhatsHot/WhatsHot.html](http://www.ca.sandia.gov/crf/WhatsHot/WhatsHot.html).



John Schmidt (left), a graduate student from the University of Arizona, Tucson, worked with Alan Kerstein this summer to develop a computational model of droplet combustion in liquid waste incinerators. The model will support a collaborative incineration research effort involving experimental and modeling work at the University of Arizona, the University of Illinois, and the Environmental Protection Agency.

## CRF hosts DOE's biopower program semi-annual review

The semi-annual review of the DOE/EE/Office of Utility Technologies Biomass Power Program was held at the CRF July 14-16. Over 60 attendees from industry, universities, national laboratories, and government participated. Highlights included an inspirational overview of the program by the DOE program managers, Ray Costello and Gary Burch, as well as technical overviews of the various research, development, and demonstration projects that constitute the program. Larry Baxter gave a detailed summary of recent CRF research on technical issues associated with cofiring of biomass and coal in utility boilers. Also included was a field trip to the nearby Tracy Biomass Plant, hosted by Andrew Carlin, Fuels Manager of the plant.

# Femtosecond photoelectron/photoion imaging probes excited molecules

The isomerization and dissociation of vibrationally excited free radicals play critical roles in determining the products of many chemical reactions important in combustion. Carl Hayden, Jeffrey LeClaire, and David Chandler, in collaboration with Julia Davies and Robert Continetti of the University of California at San Diego, are developing a novel approach to studying these processes in hot radicals. This technique combines the time resolution of femtosecond lasers with three-dimensional ion and electron imaging to probe the dynamics of highly excited molecules.

In these experiments a femtosecond laser pulse is used to photofragment precursor molecules, producing fragments with a wide range of internal energies. A single fragment is photoionized and its recoil energy determined from its arrival time and position at the ion imaging detector. From the fragment recoil energy the internal energy is calculated. The energy of the coincident electron produced in the photoionization is determined by its arrival time and position on the electron imaging detector. Collection of many coincident ions and electrons thus provides photoelectron spectra as a function of the fragment internal energy.

Recent results demonstrate the capabilities of the new apparatus. In these experiments  $\text{NO}_2$  is dissociated and ionized with 100 fs laser pulses at 372 nm. The dissociative multiphoton ionization (DMI) of  $\text{NO}_2$  is found to be a complicated process with highly correlated photoelectron and photoion distributions. The resulting  $\text{NO}^+$  ion image and arrival time distributions are shown in Figure 1.

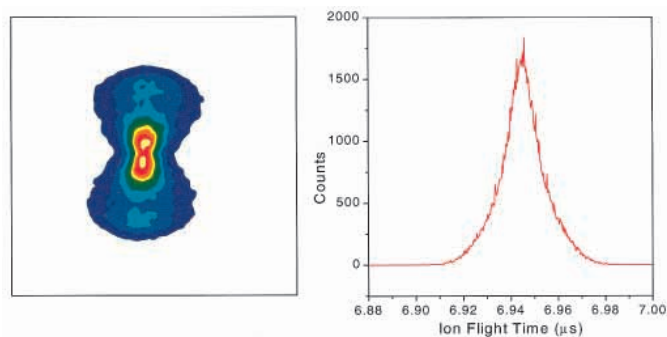


Figure 1. Ion image and arrival time distribution for  $\text{NO}^+$  from  $\text{NO}_2$  using a horizontally polarized femtosecond laser pulse at 372 nm.

Two distinct recoil energy components are observed, one with very little recoil energy, seen in the center of the image, and the second, with larger recoil energy, appearing in the larger lobes of the image. The different electron images corresponding to the slow and fast recoiling ion channels are shown in Figure 2, illustrating the measurement of photoelectron energy as a function of fragment recoil energy.

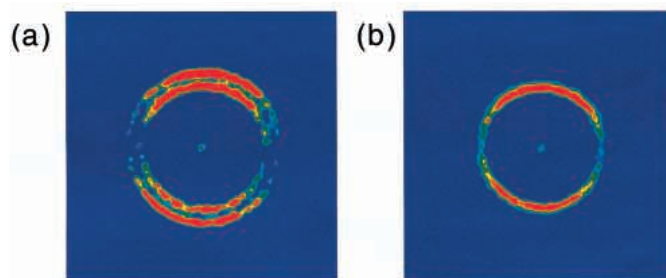


Figure 2. Coincident photoelectron images. The images are time slices through the electron spheres arriving at the detector. The electron image for slower recoiling fragments is shown in a) while the electron image for faster recoiling fragments is shown in b).

The complete correlated ion recoil and photoelectron energy distribution from DMI of  $\text{NO}_2$  is plotted in Figure 3. It can be seen that one DMI process produces  $\text{NO}^+$  in a range of vibrational states with virtually no translational energy. This process corresponds to the slow component in Figure 1 and appears as the series of peaks along the zero ion recoil energy axis. The second DMI process produces ground vibrational state  $\text{NO}^+$  with substantial recoil energy that is strongly correlated to the photoelectron energy, indicating that the electron is leaving the molecule as it is dissociating.

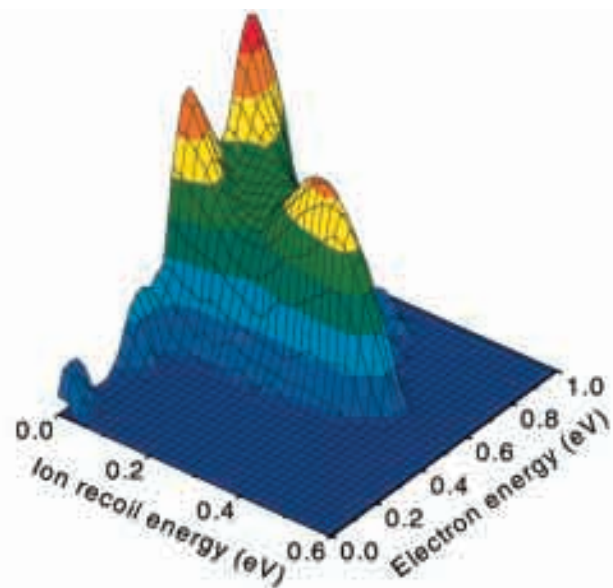



Figure 3. Plot of the photoelectron energy distribution as a function of fragment ion recoil energy for the dissociative multiphoton ionization of  $\text{NO}_2$ .

Experiments using the new apparatus for studies of isomerization in hot radicals are now under way. This new technique measures photoelectron spectra as a function of both time and radical internal energy. Since the isomeric form of a radical can be determined from its photoelectron spectrum, these experiments provide a unique means for following radical isomerization processes. 



## Energetic materials transformed to boiler fuels

Demilitarization, manufacturing defects, and degradation of energetic materials (EM) over time has resulted in a U.S. Department of Defense (DoD) stockpile of approximately 400 million tons of EM awaiting disposal. Typical disposal methods, such as open burning/open detonation, are polluting and energy-wasting. With support through a DOE/DoD Memorandum of Understanding, Steve Buckley, Gian Sclipa, Jimmy Ross, and Larry Baxter, working with Glenn Mower of Thiokol, are searching for a more environmentally friendly means of EM disposal, emphasizing resource recovery.

One means of accomplishing both objectives is desensitization of the EM and subsequent conversion to commercial boiler fuels. Power production in the boiler recovers the energy inherent in the EM, and environmental controls on the boiler mitigate pollution. The Thiokol project investigates the combustion properties of propellant used in Minuteman and Titan IV rocket motors.

Following high-pressure water washout of the rockets, Thiokol recovers the ammonium perchlorate, desensitizing the propellant. The rocket motor washout residue consists primarily of a polybutadiene rubber (40%) impregnated with aluminum flakes (55%), with approximately 5% residual ammonium perchlorate and up to 1% asbestos entrained during the washout from the motor liner. The presence of the residual chlorine and asbestos currently forces Thiokol to landfill the material as a hazardous waste, at substantial cost. The objective of this joint project is to determine whether reapplication of the washout residue as a boiler fuel is feasible, which could allow Thiokol to avoid this cost while using a more environmentally friendly disposal method.


Experiments in Sandia's Multifuel Combustor (MFC) have shown that combustion is a promising alternative to landfill disposal. At the outset of the project, the hypothesis was that the EM would encounter high enough temperatures in a boiler to melt the asbestos, effectively rendering it a non-hazard. "Asbestos" is actually any one of a number of magnesium silicates in various forms (chrysotile, riebeckite, grunerite, etc.) that,

when inhaled deeply into the lung, can result in mesothelioma, the type of lung cancer associated with asbestos exposure. Chrysotile, the most common form of asbestos, experiences both chemical and physical changes between 600°C and 1000°C that remove the health hazard; all other forms melt below 1400°C. These temperatures are easily reached in burning particles of the EM; the flame temperatures of the aluminum-containing particles are in excess of 2200°C (see figure).



Aluminum-containing rocket motor washout material exiting the MFC. White-hot particles are burning at over 2000°C.

Results from the MFC experiments are encouraging. Fly ash and deposit analyses show that when the furnace temperature is above 1000°C, all asbestos in the fuel is converted to harmless magnesium silicates. Even below 900°C, when asbestos is found in the fly ash captured at the combustor exit, all of the asbestos is associated with large (>0.5 mm characteristic size) unburned rubber particles that could never be inhaled. In other words, no inhalation danger from the asbestos has been found in the products at any temperature.

Further, FTIR analysis of the gas-phase products of combustion using a long-path cell (15.6 meter path) reveals no potentially hazardous toxic compounds such as chlorinated hydrocarbons, down to a detection limit of 5-10 ppm, at any condition in which there is excess oxygen in the furnace. These compounds are hazardous themselves and could be precursors for other hazards such as dioxins. The results show that all of the chlorine is converted to HCl, which can be easily scrubbed from the products. Pending the successful conclusion of the MFC tests, a commercial test burn will take place next year. 

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Sandia National Laboratories  
Mail Stop 9056  
P.O. Box 969  
Livermore, California 94551-0969

<http://www.ca.sandia.gov/CRF/>



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